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NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
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NEWS	17	MAR 31	LPICI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
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NEWS	24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	26	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	27	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	28	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	29	JUN 25	CA/CAPLUS and USPAT databases updated with IPC

reclassification data

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=> s dinitrotoluene (5w) nitroresol (1) prepare  
4495 DINITROTOLUENE  
285 DINITROTOLUENES

4576 DINITROTOLUENE  
 (DINITROTOLUENE OR DINITROTOLUENES)  
 296 NITROCRE SOL  
 83 NITROCRE SOLS  
 349 NITROCRE SOL  
 (NITROCRE SOL OR NITROCRE SOLS)  
 11228 PREPARE  
 1991 PREPARES  
 13175 PREPARE  
 (PREPARE OR PREPARES)  
 139238 PREP  
 2387 PREPS  
 141401 PREP  
 (PREP OR PREPS)  
 153043 PREPARE  
 (PREPARE OR PREP)  
 L1 0 DINITROTOLUENE (5W) NITROCRE SOL (L) PREPARE

=> s dinitrotoluene (L) nitro cresol  
 4495 DINITROTOLUENE  
 285 DINITROTOLUENES  
 4576 DINITROTOLUENE  
 (DINITROTOLUENE OR DINITROTOLUENES)  
 296 NITROCRE SOL  
 83 NITROCRE SOLS  
 349 NITROCRE SOL  
 (NITROCRE SOL OR NITROCRE SOLS)  
 L2 12 DINITROTOLUENE (L) NITROCRE SOL

=> d 12 1-6 ibib abs

L2 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:424704 CAPLUS

DOCUMENT NUMBER: 143:128881

TITLE: Protein engineering of the archetypal nitroarene  
 dioxygenase of *Ralstonia* sp. strain U2 for activity on  
 aminonitrotoluenes and dinitrotoluenes through  
 alpha-subunit residues leucine 225, phenylalanine 350,  
 and glycine 407

AUTHOR(S): Keenan, Brendan G.; Leungsakul, Thammajun; Smets,  
 Barth F.; Mori, Masa-aki; Henderson, David E.; Wood,  
 Thomas K.

CORPORATE SOURCE: Departments of Chemical Engineering and Molecular and  
 Cell Biology, University of Connecticut, Storrs, CT,  
 06269-3222, USA

SOURCE: Journal of Bacteriology (2005), 187(10), 3302-3310  
 CODEN: JOBAAY; ISSN: 0021-9193

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Naphthalene dioxygenase (NDO) from *Ralstonia* sp. strain U2 has not been  
 reported to oxidize nitroarom. compds. Here, saturation mutagenesis of NDO at  
 position F350 of the  $\alpha$ -subunit (NagAc) created variant F350T that  
 produced 3-methyl-4-nitrocatechol from 2,6-dinitrotoluene  
 (26DNT), that released nitrite from 2,3-dinitrotoluene (23DNT)  
 sixfold faster than wild-type NDO, and that produced 3-amino-4-methyl-5-  
 nitrocatechol and 2-amino-4,6-dinitrobenzyl alc. from 2-amino-4,6-

dinitrotoluene (2A46DNT) (wild-type NDO has no detectable activity on 26DNT and 2A46DNT). DNA shuffling identified the beneficial NagAc mutation G407S, which when combined with the F350T substitution, increased the rate of NDO oxidation of 26DNT, 23DNT, and 2A46DNT threefold relative to variant F350T. DNA shuffling of NDO nagAcAd also generated the NagAc variant G50S/L225R/A269T with an increased rate of 4-amino-2-nitrotoluene (4A2NT; reduction product of 2,4-dinitrotoluene) oxidation; from 4A2NT, this variant produced both the previously uncharacterized oxidation product 4-amino-2-nitrocresol (enhanced 11-fold relative to wild-type NDO) as well as 4-amino-2-nitrobenzyl alc. (4A2NBA; wild-type NDO does not generate this product). G50S/L225R/A269T also had increased nitrite release from 23DNT (14-fold relative to wild-type NDO) and generated 2,3-dinitrobenzyl alc. (23DNBA) fourfold relative to wild-type NDO. The importance of position L225 for catalysis was confirmed through saturation mutagenesis; relative to wild-type NDO, NDO variant L225R had 12-fold faster generation of 4-amino-2-nitrocresol and production of 4A2NBA from 4A2NT as well as 24-fold faster generation of nitrite and 15-fold faster generation of 23DNBA from 23DNT. Hence, random mutagenesis discovered two new residues, G407 and L225, that influence the regioselectivity of Rieske non-heme-iron dioxygenases.

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2005:371207 CAPLUS

DOCUMENT NUMBER: 142:413314

TITLE: Extraction of nitrocresols from wastewater produced in the manufacture of mononitrotoluene and use of the extract

INVENTOR(S): Buettner, Johannes; Allardt, Holger; Tonder, Reinhard; Reetz, Reiner; Reichelt, Michael

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 13 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037766	A1	20050428	WO 2004-EP10497	20040918
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
DE 10345601	A1	20050512	DE 2003-10345601	20030929
EP 1670745	A1	20060621	EP 2004-765388	20040918
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				

CN 1860095	A	20061108	CN 2004-80028163	20040918
JP 2007506799	T	20070322	JP 2006-529997	20040918
US 20070043244	A1	20070222	US 2006-573020	20060322
PRIORITY APPLN. INFO.:			DE 2003-10345601	A 20030929
			WO 2004-EP10497	W 20040918

AB The alkaline wastewater produced in the manufacture of O2NC6H4Me is acidified with

acids, e.g., H2SO4 and/or HNO3 to pH ≤3, and the nitroresols are extracted preferably with PhMe, o-, m- or p-O2NC6H4Me, or their mixts. The extract containing nitroresols is used as a feedstock for manufacture of dinitrotoluene.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2005:1093 CAPLUS

DOCUMENT NUMBER: 142:96315

TITLE: Phase-separation process for working up secondary components in the preparation of dinitrotoluene by the nitration of toluene

INVENTOR(S): Munnig, Jurgen; Wastian, Dietmar; Lorenz, Wolfgang; Keggenhoff, Berthold

PATENT ASSIGNEE(S): Bayer Materialsience AG, Germany

SOURCE: U.S. Pat. Appl. Publ., 4 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040267062	A1	20041230	US 2004-878079	20040628
US 6953869	B2	20051011		
DE 10329303	A1	20050203	DE 2003-10329303	20030630
EP 1493730	A1	20050105	EP 2004-14228	20040617
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
KR 2005002619	A	20050107	KR 2004-49537	20040629
CN 1576240	A	20050209	CN 2004-10063300	20040629
JP 2005023076	A	20050127	JP 2004-194526	20040630
PRIORITY APPLN. INFO.:			DE 2003-10329303	A 20030630

AB A process is described for working up organic secondary components which are formed in the one-stage or two-stage nitration of toluene to dinitrotoluene, the organic secondary components are present in the acidic and alkaline waste water from the dinitrotoluene-washing step and in the aqueous

distillate from the sulfuric acid concentration step, together with small amts. of nitrotoluene and dinitrotoluene. This process comprises: (A) combining the acidic and alkaline waste waters from the washing step and the aqueous distillate from the sulfuric acid-concentration step such that the resulting mixture has a pH <5; (B) separating the aqueous and organic phases which form by phase separation; and (C) recycling the organic phase from step (B) into the nitration process.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS

## RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:783737 CAPLUS  
 DOCUMENT NUMBER: 132:6012  
 TITLE: Dilute acid oxidation of dinitrotoluene alkaline wash water  
 INVENTOR(S): Van Court, Carr Richard; Simpson, Mark Shedric  
 PATENT ASSIGNEE(S): Air Products and Chemicals, Inc., USA  
 SOURCE: Eur. Pat. Appl., 7 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 962446	A1	19991208	EP 1998-109789	19980528
EP 962446	B1	20010801		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CN 1203904	A	19990106	CN 1998-108262	19980501
PRIORITY APPLN. INFO.:			CN 1998-108262	A 19980501
			US 1997-848933	A 19970501

AB Nitrocresols in a crude aqueous alkaline dinitrotoluene wash stream are removed using a dilute oxidizing acid such as nitric acid or sulfuric acid, heated to 130 to 180°C for a period of time required to reduce the nitrocresols to a level at which it does not precipitate from the mixed acidic wash stream at temps. above about 60°C. Removal of the remaining nitrocresols can be achieved by conventional methods such as carbon adsorption or activated sludge biotreatment. For comparison, dilute oxidizing acids are also used to treat dinitrophenols in a crude aqueous mononitrobenzene wash stream. Both 2,6-dinitrophenol and 2,4-dinitrophenol were removed, but the process was shown not to involve oxidation and picric acid was produced.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:392206 CAPLUS  
 DOCUMENT NUMBER: 129:71603  
 ORIGINAL REFERENCE NO.: 129:14755a,14758a  
 TITLE: Dilute acid oxidation of dinitrotoluene alkaline wash water  
 INVENTOR(S): Van Court Carr, Richard; Simpson, Mark Shedrick  
 PATENT ASSIGNEE(S): Air Products and Chemicals, Inc., USA  
 SOURCE: U.S., 4 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5762802	A	19980609	US 1997-848933	19970501

BR 9801469                   A       20000208       BR 1998-1469                   19980428  
 CN 1203904                   A       19990106       CN 1998-108262               19980501  
 PRIORITY APPLN. INFO.:       US 1997-848933               A   19970501  
 AB   A process for removing nitroresols in a crude aqueous alkaline  
      dinitrotoluene wash stream derived by nitration of toluene using a  
      mixed acid technique followed by treatment with aqueous alkaline material in  
 which  
      the crude aqueous alkaline dinitrotoluene wash stream is mixed with a  
      dilute oxidizing acid such as nitric acid, heated to 130° to  
      180°. for a period of time required to reduce the  
      nitroresols to a level at which it does not precipitate from the mixed  
      acidic wash stream at temps. above about 60°, and removing the  
      remaining nitroresols by conventional methods such as  
      adsorption or activated sludge biotreatment.  
 REFERENCE COUNT:           11       THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS  
    RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2   ANSWER 6 OF 12   CAPLUS   COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER:       1987:611289   CAPLUS  
 DOCUMENT NUMBER:       107:211289  
 ORIGINAL REFERENCE NO.:   107:33731a,33734a  
 TITLE:               Spectrophotometric determination of dinitroresol in  
                       industrial dinitrotoluene  
 AUTHOR(S):           Wang, Zhaoxing; Fu, Ruonong  
 CORPORATE SOURCE:     Dep. Chem. Eng., Beijing Ind. Coll., Beijing, Peop.  
                       Rep. China  
 SOURCE:               Fenxi Huaxue (1987), 15(7), 670  
                       CODEN: FHHHDT; ISSN: 0253-3820  
 DOCUMENT TYPE:       Journal  
 LANGUAGE:           Chinese  
 AB   Dinitroresol in industrial dinitrotoluene was extracted with dilute KOH  
      solution,  
      followed by addition of a known amount of standard 2-methyl-3,5-dinitrophenol  
 or  
      4-methyl-3,5-dinitrophenol. The dinitroresol was determined by measuring the  
      absorbance at 436 nm vs. the same solution which was acidified with 6M HCl.  
      Beer's law was obeyed for dinitroresol at  $2.5 \times 10^{-3}$  -  $2.5 \times$   
       $10^{-2}$  mg/mL. The relative standard deviation was <1% in the determination of  
 0.002%  
      dinitroresol in dinitrotoluene. The recovery of dinitroresol was >95%.

=> d 12 7-12 ibib abs

L2   ANSWER 7 OF 12   CAPLUS   COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER:       1986:539142   CAPLUS  
 DOCUMENT NUMBER:       105:139142  
 ORIGINAL REFERENCE NO.:   105:22363a,22366a  
 TITLE:               Removal of nitroresols from  
                       dinitrotoluene waste streams using Fenton's  
                       reagent  
 INVENTOR(S):          Carr, Richard V. C.; Martin, Carl J.; Gonzalez,  
                       Roland; Albanese, Thomas A.  
 PATENT ASSIGNEE(S):   Air Products and Chemicals, Inc., USA  
 SOURCE:               U.S., 4 pp.  
                       CODEN: USXXAM  
 DOCUMENT TYPE:       Patent

LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4604214	A	19860805	US 1985-766849	19850816

PRIORITY APPLN. INFO.: US 1985-766849 19850816  
 OTHER SOURCE(S): MARPAT 105:139142

AB Nitrocresols and picric acid are removed from wastewaters from nitroaroms. production, e.g. dinitrotoluene, by washing the crude product with alkaline medium, e.g. Na<sub>2</sub>CO<sub>3</sub>, NH<sub>4</sub>OH, NaOH, NaHCO<sub>3</sub>, or KOH, until concentration of the water-soluble trinitrocresol and picric acid salts is sufficiently high, reducing the pH of the wastewater to 3-4 using aqueous acid, e.g., H<sub>2</sub>SO<sub>4</sub> or HNO<sub>3</sub>, and then adding H<sub>2</sub>O<sub>2</sub> and Fe<sup>2+</sup> to oxidize the trinitrocresol to carboxylic acid, HNO<sub>3</sub>, and CO<sub>2</sub>. The Fe<sup>2+</sup> may be FeSO<sub>4</sub>.

L2 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1986:465887 CAPLUS  
 DOCUMENT NUMBER: 105:65887  
 ORIGINAL REFERENCE NO.: 105:10655a,10658a  
 TITLE: Precipitative removal of nitrocresols from dinitrotoluene waste streams  
 INVENTOR(S): Carr, Richard V. C.; Sawicki, John E.; Toseland, Bernard A.  
 PATENT ASSIGNEE(S): Air Products and Chemicals, Inc., USA  
 SOURCE: U.S., 4 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4597875	A	19860701	US 1985-731424	19850507

PRIORITY APPLN. INFO.: US 1985-731424 19850507  
 OTHER SOURCE(S): MARPAT 105:65887

AB An alkaline wash water containing water soluble nitrocresols and picric acid from the manufacture of dinitrotoluene is recycled through the wash process and then treated with aqueous acid to precipitate the orgs. The orgs. are removed and incinerated. Thus, wash water that contained 1.13 weight% trinitrocresols was adjusted to pH 1 with H<sub>2</sub>SO<sub>4</sub>. The liquid precipitate contained 88% of the orgs. and was removed and incinerated.

L2 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1986:38945 CAPLUS  
 DOCUMENT NUMBER: 104:38945  
 ORIGINAL REFERENCE NO.: 104:6310h,6311a  
 TITLE: A continuous stirred tank reactor investigation of the gas-phase reaction of hydroxyl radicals and toluene  
 AUTHOR(S): Gery, Michael W.; Fox, Donald L.; Jeffries, Harvey E.; Stockburger, Leonard; Weathers, Walter S.  
 CORPORATE SOURCE: Sch. Public Health, Univ. North Carolina, Chapel Hill, NC, 27514, USA



SOURCE: International Journal of Chemical Kinetics (1985),  
17(9), 931-55  
CODEN: IJCKBO; ISSN: 0538-8066

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A continuous stirred tank reactor (CSTR) was used to study the gas-phase reaction between OH radicals and PhMe [108-88-3]. The OH radicals were generated by the in-situ photolysis of HNO<sub>2</sub>. Flow reactor operation at steady-state conditions with a residence time of 20 min allowed investigation of primary and very rapid secondary reactions. CSTR and batch reactor expts. were also performed with selected products. Both gas-phase and aerosol products were identified by chromatog. and mass spectroscopy, with total product yields between 55 and 75% of reacted C. PhMe reaction products included cresols, nitrocresols, nitrotoluenes, 3,5-dinitrotoluene [618-85-9], benzaldehyde [100-52-7], benzyl nitrate [15285-42-4], methyl-p-benzoquinone [553-97-9], glyoxal [107-22-2], methylglyoxal [78-98-8], HCHO [50-00-0], peroxyacetyl nitrate [2278-22-0], CO, and nitrophenols. The fraction of abstraction of Me H atoms by OH radicals was calculated to be 0.13 ± 0.04. The ratio of reaction rate consts. for nitrotoluene vs. cresol formation from the HO adduct was calculated to be .apprx.3.3 + 104. Also, the ratio of cresol formation vs. O<sub>2</sub> addition to the HO adduct was estimated to be ≥0.5 for atmospheric conditions. Comparisons of these measurements with previous values and the implications with respect to photochem. kinetic modeling of the atmospheric are discussed.

L2 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:576631 CAPLUS

DOCUMENT NUMBER: 101:176631

ORIGINAL REFERENCE NO.: 101:26656h,26657a

TITLE: Atmospheric reactions of o-cresol: gas phase and aerosol products

AUTHOR(S): Grosjean, Daniel

CORPORATE SOURCE: Environ. Res. and Technol., Inc., Westlake Village, CA, 91361, USA

SOURCE: Atmospheric Environment (1967-1989) (1984), 18(8), 1641-52  
CODEN: ATENBP; ISSN: 0004-6981

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Photochem- oxidation of o-cresol [95-48-7] (0.5-1.0 ppm) and NO<sub>x</sub> (0.12-0.66 ppm) in air yielded the following gas-phase products: pyruvic acid [127-17-3], AcH [75-07-0], HCHO [50-00-0], peroxyacetyl nitrate [2278-22-0], nitrocresol [12167-20-3] and trace levels of HNO<sub>3</sub> and methyl nitrate [598-58-3]. Particulate phase products included 2-hydroxy-3-nitrotoluene [13073-29-5], 2-hydroxy-5-nitrotoluene [99-53-6], 2-hydroxy-3,5-dinitrotoluene [534-52-1] and, tentatively, several hydroxy-nitrocresol isomers. Yields of gas-phase products (0.8% for pyruvic acid, 5-11% for the sum of the aromatic ring fragmentation products) and of aerosol products (5-19% on a C basis, with particulate C formation rates of 30-80 µg/m<sup>3</sup>-h) are discussed in terms of photochem. reaction pathways. From 60 to 89% of the initial NO<sub>x</sub> was consumed in these reactions, and a significant fraction of the reacted NO<sub>x</sub> could be accounted for as particulate nitroarom. products.

L2 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1916:4978 CAPLUS

DOCUMENT NUMBER: 10:4978  
 ORIGINAL REFERENCE NO.: 10:967f-i,968a-d  
 TITLE: Trinitrotoluene  
 AUTHOR(S): Copisarow, M.  
 SOURCE: Chemical News and Journal of Industrial Science  
 (1915), 112, 247-8  
 CODEN: CHNWAY  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB cf. following abstract. Six isomers of trinitrotoluene are known:  $\alpha$ -, 2, 4, 6, m. 80.8°;  $\beta$ -, 2, 3, 4, m. 112°;  $\gamma$ -, 2, 4, 5, m. 104°;  $\delta$ -, 3, 4, 5, m. 137-5°;  $\epsilon$ -, 2, 3, 5, m. 97.2°;  $\zeta$ -, 2, 3, 6, m. 79-5°. Com. trinitrotoluene, while principally the  $\alpha$ -form, is accompanied by other modifications, produced from m-nitrotoluene, which constitute about 4.5% of the com. mononitrotoluene. All of the isomers of trinitrotoluene are of practically the same value as explosives. They may be distinguished by acetone and  $\text{NH}_3$  with which the  $\alpha$ -form gives deep red,  $\beta$ -form. greenish yellow,  $\gamma$ -form blue,  $\epsilon$ -form rose-red and the  $\zeta$ -form orange-red. The manufacture of trinitrotoluene is usually carried out in 2 or 3 stages, the concentration of acids being gradually increased, and although by itself a simple process, numerous chemical and technical difficulties are met with when the manufacture is conducted on a large scale. Chief among these is the presence in the product of inorganic impurities derived from Pb compds. in the acids or from the action of the acids on the apparatus in which the nitration is carried out, and of organic intermediate compds. and by-products due to imperfect stirring, to concentration and ratio of acid and to duration and temperature of reaction. A check on the operation may be found in the appearance and analysis of the spent acid which varies in color from yellowish to dark brown, the color being the darker the less the nitric and the more the sulfonic acids, as well as organic matter, present. The mineral matter present during the process may act either as a catalyst or a chemical reagent. When the mineral acids act upon the metal parts of the apparatus H may be set free and it may reduce some of the nitro compds. Under the working conditions amino groups may be diazotized yielding cresols and nitrocresols whose salts are highly sensitive explosives and thus there may be obtained as by-products: (1) trinitrobenzoic acid, and even tetranitromethane, owing to oxidation in case of overheating or pressure. The intense odor of the latter is sometimes observed in the factories, but the former, owing to its solubility, generally escapes detection; (2) phenolic compds., like cresols, owing to the reduction of some of the nitro compds.; (3) sulfonic acids, when the quantity of nitric in the mixed acid is below the minimum. In the process of manufacture of trinitrotoluene the following must be observed: (1) The amount of  $\text{HNO}_3$  to be used must exceed at least by 1/2 mol. the quantity theoretically required for the carrying out of the nitration to a certain stage. (2) The extent of nitration should be regulated more by the concentration of the acids, temperature, and duration of reaction than by the actual quantity of  $\text{HNO}_3$  present. (3) The reaction product should not be kept in contact with the spent acid longer than is really unavoidable. (4) The concentration of acid and material of plant should be such as to reduce their action on one another to a minimum. (5) The starting materials (toluene and acids) must be pure. The residue from the mother-liquors consists of a complex mixture of various di- and trinitrotoluenes. By nitrating this with a mixed acid containing only 15% of  $\text{HNO}_3$  a "liquid

trinitrotoluene" is obtained, which has considerable power, and has the property of gelatinizing collodion cotton, as nitroglycerin does. It is used in the manufacture of gelatinized explosives. It contains 16.6 to 17.2% of N, whereas pure trinitrotoluene contains 18.5% and dinitrotoluene 15.4%. Other details of importance to manufacturers and users of trinitrotoluene are set forth.

L2 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1906:40356 CAPLUS

DOCUMENT NUMBER: 0:40356

TITLE: On orcinol and some of the other dihydroxytoluenes

AUTHOR(S): Neville, R. H. C.; Winther, A.

SOURCE: Journal of the Chemical Society, Transactions (1882), 41, 415-428

From: J. Am. Chem. Soc. 5(4), 61-2 1883

CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Believing that Orcinol was a dihydroxytoluene, the authors undertook this investigation. Taking dinitroparatoluene 1:3:5 made from dinitropartoluidine, it was dissolved in alcohol and treated with ammonium sulphide. Water was added and the precipitate dissolved in hydrochloric acid and reprecipitated with ammonia. By further purification thick needles of nitrotoluidine were obtained melting at 98°-98°.4. The yield was 50 percent of the dinitrotoluene used. By treating with sulphuric acid the sulphate was obtained; which by further treatment with potassic nitrite gave nitrocresol as a brown oil, which by purification with ether gave yellow needles of nitrocresol. The nitrocresol was treated with tin and hydrochloric acid; after removing the tin, the solution was evaporated, and the crystals obtained washed with ether to remove unreduced nitrocresol. From this chloride dihydroxytoluene is obtained by treating with sulphuric acid and potassic nitrite. The resulting oil purified by distillation and crystallizing from benzene and chloroform, gives from the first needles or prisms and from the latter white leaves. After 14 days over sulphuric acid it melts at 106°-108°; which by analysis proves to be orcinol C<sub>6</sub>H<sub>3</sub>.CH<sub>3</sub>, (OH)<sub>2</sub> 1:3:5. The authors have also succeeded in making orcinol from metabromo-toluene-metasulphonic acid; toluene-meta-disulphonic acid; metabromo-metatoluidine; metadibromotoluene. During this research the authors have also obtained the dihydroxytoluene 1:2:4, starting with orthonitro-paratoluidine. This latter was converted in sulphate, treated with potassic nitrite and converted into nitrocresol. This nitrocresol was treated with tin and hydrochloric acid to obtain amido-cresol. The chloride of amido-cresol thus obtained by treatment with sulphuric acid and potassic nitrite and the dihydroxytoluene obtained as an oil, which afterward crystallized, and by sublimation and crystallization gave a melting point of 104°-105°. The author also prepared dihydroxytoluene 1:2:5 from meta-nitro-orthotoluidine following nearly the same process as in above case. The dihydroxytoluene 1:2:5 obtained is in white leaves melting at 124°-125° and freely soluble in alcohol, ether or water. An investigation of the dihydroxytoluene 1:3:4 was also made by the authors starting with metanitro-paratoluidine, following the method above used by preparing the diazo compound, but was unsatisfactory. The method of Wagner (Ber. 1874, 537) was used, and by slight modification with success. The paper is a very lengthy one and filled with most interesting details in manipulation of the methods used.

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L1 0 S DINITROTOLUENE (5W) NITROCRESOL (L) PREPARE

L2 12 S DINITROTOLUENE (L) NITROCRESOL

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